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MONTE CARLO SIMULATIONS OF FERMION SYSTEMS: THE DETERMINANT METHOD

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Described are the details for performing Monte Carlo simulations on systems of fermions at finite temperatures by use of a technique called the Determinant Method. This method is based on a functional integral formulation of the fermion problem [Blankenbecler et al., Phys. Rev. D 24, 2278 (1981)] in which the quartic fermion-fermion interactions that exist for certain models are transformed into bilinear ones by the introduction [J. Hirsch, Phys. Rev. B 28, 4059 (1983)] of Ising-like variables and an additional finite dimension. It is on the transformed problem the Monte Carlo simulations are performed. A brief summary of research on two such model problems, the spinless fermion lattice gas and the Anderson impurity problem, is also given.

MONTE CARLO SIMULATIONS OF FERMION SYSTEMS: THE DETERMINANT METHOD

INTRODUCTION

In the past several years an upswell in interest and activity in performing Monte Carlo simulations of systems obeying the laws of quantum mechanics has occurred. Causing this upswell is both the development of algorithms for performing the simulations and the availability of computers big and fast enough to make the use of such algorithms practical. Indeed for some problems the use of a CRAY-like computer is essential.

In contrast to classical statistical mechanics, where the phase "Monte Carlo simulations" refers still to the method developed by Metropolis et al., in quantum statistical mechanics there are several quite distinct Monte Carlo methods. There is a variational method, Green's function method, path-integral method, determinant method, etc. Although each method has the importance sampling concept expressed by Metropolis et al. at its core, their details, and the basis for their details, are often distinct. For example, the methods work either at zero temperature or finite temperature, but not both. Often they work well for bosons but require supplementary procedures to work for fermions. The subject of this paper, the determinant method,[2,3] works for fermions at finite temperatures, although it is rooted in an approach that allows the simulations of fermions, bosons and their interactions.

Our description of the determinant method will develop in several stages. First, we will present a broad view of its major parts. Emphasis will be on the introduction of additional degrees of freedom to transform the original quantum calculation into a calculation involving classical degrees of freedom. Then details to the major parts will be added. Following this, several points useful for its implementation are discussed. Next an illustration is given of how various thermodynamic and correlation functions are calculated. Then, in conclusion, we present a very brief description of the results of simulating the properties of the spinless fermion lattice gas[4] and Anderson impurity model.[5]

BASIC IDEA

What one wants to evaluate are thermodynamic averages of different physical quantities. Such an average for a typical quantity A is defined by

$$\langle A \rangle = \frac{\mathrm{Tr}\, e^{-\beta H}}{Z} \tag{1}$$

where the partition function Z is

$$Z = \mathrm{Tr}\, e^{-\beta H} \tag{2}$$

The problem is in general the inability not only to exponentiate the quantum hamiltonian but also to perform the required trace. To mitigate these problems, we make an approximation that introduces additional degrees of freedom and an extra (finite) dimension into the problem. The approximation is controlled in the sense that the error in principle can be made as small as we like. For each configuration of these new variables the approximation corresponds to replacing the original hamiltonian by an effective one for which we can perform the trace over the original (i.e. the fermion) degrees of freedom. Symbolically, we have

$$\langle A \rangle \simeq \frac{\mathrm{Tr}_\sigma \, \mathrm{Tr} A e^{-\beta h[\sigma]}}{\mathrm{Tr}_\sigma \mathrm{Tr} e^{-\beta h[\sigma]}} \tag{3}$$

$$= \frac{\mathrm{Tr}_\sigma z[\sigma] [z[\sigma]^{-1} \mathrm{Tr} A e^{-\beta h[\sigma]}]}{\mathrm{Tr}_\sigma z[\sigma]} \tag{4}$$

$$= \frac{\mathrm{Tr}_\sigma A(\sigma) z[\sigma]}{\mathrm{Tr}_\sigma z[\sigma]} \tag{5}$$

where σ represents a configuration of the new degrees of freedom and

$$z[\sigma] = \mathrm{Tr} e^{-\beta h[\sigma]} \tag{6}$$

is the partition function of the configuration-dependent effective hamiltonian. It is the average represented by (5) that is done by the Monte Carlo methods; however, instead of using the standard statistical probability density $e^{-\beta H}/Z$ we now must use $z[\sigma]/Z$. It is in $z[\sigma]$ where the quantum mechanical details are embodied.

SOME DETAILS

THE TROTTER APPROXIMATION

To add details of the method, we focus on the partition function. The first step is to introduce a small parameter τ into the problem. Because the hamiltonian always commutes with itself, we can write

$$Z = \mathrm{Tr} \, e^{-\beta H}$$

$$= \mathrm{Tr} \, e^{-\tau H} e^{-\tau H} \ldots e^{-\tau H} \tag{7}$$

with $\tau = \beta/L$ where L is the number of $e^{-\tau H}$ factors is the argument of the trace. We now approximate $e^{-\tau H}$. To do this we note that

$$H = H_0 + H_I$$

where H_0 is the non-interacting part of the hamiltonian, which is quadratic in the fermion degrees of freedom, and H_I is the interacting part, which for the models we consider is quartic in the fermion degrees of freedom. Since H_0 and H_I do not commute we use the Trotter approximation[6] to write

$$e^{-\tau H} \simeq e^{-\tau H_0} e^{-\tau H_I} + O(\tau^2)$$

Hence we in principle can make this a very good approximation by making τ small. Having done this, we have a piece $\exp(-\tau H_0)$ which generally is easily evaluated, but are still faced with exponentiating H_I. This step is accomplished for certain models by using a form of the Hubbard-Stratanovich transformation.[6]

THE HUBBARD-STRATANOVICH TRANSFORMATION

This transformation is best illustrated by an example. For our example we choose the Hubbard hamiltonian

$$H = -t \sum_{<ij>s} (c^{+}_{is} c_{js} + c^{+}_{js} c_{is}) + U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{8}$$

where i refers to a lattice site, $<ij>$ to a nearest neighbor pair of sites, s to a up or down spin, where $n_{is} = c^{+}_{is} c_{is}$ is the fermion number operator, and c^{+}_{is} and c_{is} are fermion creation and destruction operators. For this hamiltonian

$$H_I = U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{9}$$

The transformation uses the following identity[3]

$$e^{-\tau U n_{i\uparrow} n_{i\downarrow}} = \frac{1}{2} \sum_{\sigma_i(\ell)=\pm 1} e^{-\tau J \sigma_i(\ell)(n_{i\uparrow} - n_{i\downarrow}) - \tau U/2 (n_{i\uparrow} + n_{i\downarrow})}$$

with $\cosh \tau J = e^{\tau U/2}$, which is applied to each site in (9) and to each factor in (7). If the sites are arranged in a two-dimensional lattice, at each site

we have an Ising spin at L sites in a third dimension. From more formal approaches to the problem this third dimension corresponds to an imaginary time axis obtained by the change of variable $it = (kT)^{-1}$. Additionally factors in (7) then corresponds to a different time steps of the problem. For convenience in the following we will use this "time" terminology.

From (10) we see that the term in (8) quartic in the creation and destruction operators has been replaced by one that is quadratic: The orginal H in the ℓth factor of (7) has been replaced by an $H(\ell)$ that is non-interacting and hence its exponential form is treatable by standard means. In particular we define

$$H(\ell) \equiv \sum_{ijs} c^{+}_{is} h^{s}(\ell) c_{js}$$

We can now rewrite (7) as

$$Z = Tr_{\sigma}\, Tr e^{-\tau H(1)} e^{-\tau H(2)} \cdots e^{-\tau H(L)} \tag{10}$$

and because of quartic form of $H(\ell)$ we can trace out the fermion degrees of freedom to obtain

$$Z = Tr_{\sigma}\, \det(I + B_1 B_2 \cdots B_L)$$

$$= Tr_{\sigma}\, \det(I + B_2 \cdots B_L B_1)$$

etc

$$= Tr_{\sigma} z[\sigma]$$

where

$$B_{\ell} = e^{-\tau h(\ell)}$$

and

$$z[\sigma] = \det(I + B_{\ell} \cdots B_1 B_L \cdots B_{\ell+1}) \tag{11}$$

is the partition function associated with a given configuration of the Ising-like variables.

THE GREEN'S FUNCTION

For every time step ℓ, the Monte Carlo procedure consists of going from site to site and deciding whether to accept or reject a spin flip. The decision is generally based on the Metropolis or heat bath algorithms. However in contrast to classical statistical mechanics where one examines the ratio

$$e^{-\beta H[\sigma']}/e^{-\beta H[\sigma]}$$

we must examine

$$z[\sigma']/z[\sigma]$$

The evaluation of $z[\sigma]$ generally involves $(L+1)n^3$ multiplications where N is the number of degrees of freedom in the original problem. To reduce the computation time, the following alternatives have been devised: The cyclic properties of the products of the B's presented in (11) are used so at the ℓth time step

$$z[\sigma] = \det(I + B_{\ell+1} \cdots B_2 B_1 \cdots B_\ell) \tag{12}$$

Then for a new configuration we write the new B_ℓ as $B_\ell \Delta_\ell$. Hence

$$\frac{z[\sigma']}{z[\sigma]} = \frac{\det(I + B_{\ell+1} \cdots B_L B_1 \cdots B_\ell \Delta_\ell)}{\det(I + B_{\ell+1} \cdots B_L B_1 \cdots B_\ell)}$$

Defining

$$g_\ell = (I + B_{\ell+1} \cdots B_L B_1 \cdots B_\ell)^{-1} \tag{13}$$

we can reexpress the ratio by

$$\det[I + (g_\ell - I)(\Delta_\ell - I)] \tag{14}$$

When the interactions are short ranged, $\Delta_\ell - I$ is a sparse matrix and (14) can generally be evaluated with operations of the order N^2, N, or 1, provided g_ℓ is known.

On the surface g_ℓ requires as many operations to compute as the original determinant. However there are several useful relations which allows the operation count to be reduced. The first generates a new g'_ℓ from the g_ℓ whenever the configuration changes. Starting with

$$g'_\ell = (I + B_{\ell+1}\ldots B_L B_1 \ldots B_\ell \Delta_\ell)^{-1}$$

one can show

$$g'_\ell = g_\ell - (I-g_\ell)(\Delta_\ell - I)g'_\ell \tag{15}$$

Because of the sparseness of $(\Delta_\ell - I)$ the equation can usually be solved for g'_ℓ in as few as $O(N^2)$ operations.

We also have a procedure to go from one time to another more efficiently then by constructing the appropriate g from (13). It is

$$g_{\ell+1} = B_\ell g_\ell B_\ell^{-1} \tag{16}$$

The main point is after having made g_1 via (13) at the very start of the simulation we in principle can generate all other g_ℓ's in considerable few operations via (15) and (16) than by (13). In practice errors build-up and so to maintain an acceptable level of precision (13) is used, from time to time, to control these errors.

The functions g_ℓ instead of $z[\sigma]$ are the principal quantities needed and computed in the simulations. This is some sense is a fortunate circumstance, for one can show[2-4]

$$[g_\ell]_{ij} = g_{ij}(\ell-1,\ \ell-\ell)$$

where g_{ij} is the following thermodynamic (or equal time) Green's function[8]

$$g_{ij}(\ell^+,\ell) = \langle c_i(\ell)\ c_j^+(\ell)\rangle$$

Here ℓ implies $\ell\tau$ and ℓ^+, $\ell\tau+\varepsilon$ with $0 < \varepsilon \ll 1$. Similarly one can show

$$\langle n_i(\ell)\rangle = 1 - g_{ii}(\ell^+,\ell)$$

and also find specific expressions[2,4] for the unequal time Green's functions $g_{ij}(\ell,m)$ in terms of products of the B_ℓ's.

COMPUTER QUANTITIES

The Green's function is the principal product of our simulation. With it and the use of Wick's theorem, we are able to compute all relevant thermodynamic and many-body correlation functions. Quantities computed by this method

include: the energy, specific heat, magnetic susceptibility, singlet superconducting susceptibility, density-density correlation function, the polarizibility, etc. To illustrate the procedure, we will now sketch the computation of the average energy for the Hubbard hamiltonian.

$$E = \langle H \rangle$$

From (8) we see averages like $\langle c^{+}_{is} c_{js} \rangle$ and $\langle n_{i\uparrow} n_{i\downarrow} \rangle$ are needed. Since in (8) $i \neq j$, $\langle c^{+}_{is} c_{js} \rangle = - \langle c_{is} c^{+}_{js} \rangle$ which is just g^{s}_{ij}. To do the other type of average, we must use Wick's theorem:[8]

$$\langle n_{i\uparrow} n_{i\downarrow} \rangle = \langle c^{+}_{i\uparrow} c_{i\uparrow} c^{+}_{i\downarrow} c_{i\downarrow} \rangle$$

$$= \langle c^{+}_{i\uparrow} c_{i\uparrow} \rangle \langle c^{+}_{i\downarrow} c_{i\downarrow} \rangle + \langle c_{i\downarrow} c^{+}_{i\uparrow} \rangle \langle c_{i\uparrow} c^{+}_{i\downarrow} \rangle$$

The averages in the first term on the right-hand side are just $\langle n_{is} \rangle = 1 - g^{s}_{ii}$. Those in the last term are zero! The Hubbard-Stratanovich transformation took term with explicit interactions between opposite spins and replaced it with one that produces an effective hamiltonian block diagonal in s. For purposes of computing $\langle c^{+}_{i\uparrow} c_{i\downarrow} \rangle$ etc. there are no correlations between spins so such averages are zero. The spins correlations remain only implicitly: the spins interact through the Ising spin field which may be regarded as an imaginary-time dependent, external random field that is summed over all possible configurations.

RESEARCH SUMMARY

To date, using the determinant method, we have performed quantum Monte Carlo simulations on two models: the spinless Fermion lattice gas and the Anderson impurity problem. Work on the first model was recently completed; work on the second was recently started.

SPINLESS FERMION LATTICE GAS

For a half-filled band the hamiltonian for this model is [3]

$$H = - t \sum_{\langle ij \rangle} (c^{+}_{i} c_{j} + c^{+}_{j} c_{i}) + V \sum_{\langle ij \rangle} (n_{i} - \tfrac{1}{2})(n_{j} - \tfrac{1}{2})$$

As in the Hubbard model c^{+}_{i} and c_{i} are fermion creation and destruction operators and $n_{i} = c^{+}_{i} c_{i}$ is the fermion number operator. In the model, spinless fermions hop on a two-dimensional lattice with a nearest neighbor interaction V. RPA calculations predict that the half-filled system undergoes a density-wave transition for $V > 0$, an odd angular momentum pairing transition for small negative V, and a condensation transition for more negative values of V. The

Ising limit matches onto the density wave transition for $V > 0$ and onto the condensation transition for $V < 0$. A strong coupling expansion provides the leading corrections to the Ising limit. The intermediate coupling regime was explored by the Monte Carlo simulations and various Green's functions characterizing the quantum correlations were evaluated. Then, using finite size scaling techniques, we determined the density wave and condensation phase boundaries. At these transitions, measured quantities scaled well with the usual Ising indices. Unfortunately, the weak coupling regime lies beyond the reach of our simulations.

ANDERSON IMPURITY MODEL

The hamiltonian for this model is[5]

$$H = \sum_{ks} [E_k n_{ks} + V_{kf}(c^+_{ks}c_{fs} + c^+_{fs}c_{ks})]$$

$$+ E_f(n_{f\uparrow} + n_{f\downarrow}) + Un_{f\uparrow}n_{f\downarrow}$$

Here electrons exist in a band described by E_k or an impurity (f-level) state with energy E_f. The band and impurity interact with energy V_{kf}, and if two electrons try to occupy the impurity level they experience a Coulomb repulsion of strength U. This model admits a variety of possible physical phenomena including local magnetic moment formation, valence fluctuations, Kondo effect, etc., and is commonly used to describe the properties of rare earth and actinide materials.

The code for this simulation is written and tested for several very simple cases. We are presently using the code to see how much of the Bethe-ansatz solution[9] to the Anderson impurity model can be reproduced. In this solution E_k is assumed to vary linearly with k. We have no results yet.

CONCLUDING REMARKS

We have presented an introductory description of the determinant method with several important details for its practical implimentation. For more details the Blankenbecker et al.,[2] the Hirsch,[3] and the appendix of the Gubernatis et al.[4] papers should be consulted. The latter also gives many detailed results for the spinless Fermion lattice gas and useful ways to interpret the data. Similar details for the Hubbard model are given in reference 3.

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